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氢原子波函数的玻色算子表示*

李兴华† 杨亚天
(福建师范大学物理与光电信息科技学院, 福州 350007)
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用四类玻色算子及博戈留波夫(Bogoliubov)变换,统一给出了氢原子波函数的表达式,并讨论了它们和波函数球坐标表达式的对应关系,完满地解决了氢原子波函数的算子表示问题.

关键词:玻色算子, 氢原子, 波函数
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1. 引 言

三维各向同性谐振子(3DIHO)和氢原子(HA)都是典型的可积系统,相应的量子力学问题有直接求解微分方程的波动力学解法和代数解法[1—9]. 代数解法又有两种,一种是对径向解引入与角动量量子数 l 有关的四类升降算子法[5—9],另一种是采用具有角动量性质的玻色算子法[10]. 对 3DIHO 的波函数,其李代数比较简单,波函数有简明统一的表达式. 对 HA 的波函数,本文引入四类玻色子构成的角动量算子进行表述. 这种表述方法先前虽出现过[9],但先前的代数解法只解出能谱公式,没有波函数的一般表述,而且这些玻色子跟坐标及其微分算子的关系也未讨论. 本文除给出能谱关系外,还解决了后两个问题.

必需指出, HA 比 3DIHO 要复杂得多,虽然波函数有统一的表述方式,但标度因子却是依赖频率(或能量)的,本文用一套基态玻色算子外加一个 Bogoliubov 变换,解决了这个问题,得到氢原子波函数的简洁表达式.

2. 氢原子能量本征值

由 Kus tan nheimo-Stiefel 变换[11]

$$r_1 = 2(s_1 s_3 - s_2 s_4),$$
$$r_2 = 2(s_1 s_4 + s_2 s_3),$$
$$r_3 = s_1^2 + s_2^2 - s_3^2 - s_4^2, \tag{1}$$

氢原子定态薛定谔方程 $\left[-\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{r}\right]\psi = E\psi$ 可化为[12]

$$\left[-\frac{\hbar^2}{2M}\Box_s + \frac{1}{2}M\omega_E^2 s^2\right]\psi = \varepsilon\psi, \tag{2}$$

其中 $M = 4m$, $\varepsilon = e^2$, $\omega_E = \left(-\frac{2E}{M}\right)^{1/2}$, 并有

$$r = (r_1^2 + r_2^2 + r_3^2)^{1/2} = \sum_{\mu=1}^{4} s_\mu^2 \equiv s^2,$$
$$\nabla^2 = \frac{1}{4r}\sum_{\mu=1}^{4}\frac{\partial^2}{\partial s_\mu^2} \equiv \frac{1}{4r}\Box_s. \tag{3}$$

设 s_μ 的共轭动量 $\pi_{s\mu} = -i\hbar\frac{\partial}{\partial s_\mu}$, 引入变换 $\eta_\mu = \sqrt{\frac{M\omega_E}{\hbar}}s_\mu$, $\pi_\mu = \frac{\pi_{s\mu}}{\sqrt{M\omega_E\hbar}}$, 并记生灭算子 τ_μ^+, $\hat{\tau}_\mu$

$$\tau_\mu^+ = \frac{1}{\sqrt{2}}(\eta_\mu - i\pi_\mu) = \frac{1}{\sqrt{2}}\left(\eta_\mu - \frac{\partial}{\partial\eta_\mu}\right),$$
$$\hat{\tau}_\mu = \frac{1}{\sqrt{2}}(\eta_\mu + i\pi_\mu) = \frac{1}{\sqrt{2}}\left(\eta_\mu + \frac{\partial}{\partial\eta_\mu}\right). \tag{4}$$

令 $\hat{n}_\mu = \tau_\mu^+\hat{\tau}_\mu$, 则[13]

$$h_E \equiv -\frac{\hbar^2}{2M}\Box_s + \frac{1}{2}M\omega_E^2 s^2 = \sum_\mu \hbar\omega_E\left(\hat{n}_\mu + \frac{1}{2}\right). \tag{5}$$

(2)式可化为

$$h_E|n_{\tau\mu}\rangle = \hbar\omega_E(n_\tau + 2)|n_{\tau\mu}\rangle = \varepsilon|n_{\tau\mu}\rangle, \tag{6}$$

其中 $|n_{\tau\mu}\rangle \equiv |n_{\tau1}n_{\tau2}n_{\tau3}n_{\tau4}\rangle$, $\hat{n}_\mu|n_{\tau\mu}\rangle = n_{\tau\mu}|n_{\tau\mu}\rangle$, n_τ

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† E-mail: xhli1@mail.china.com

$=\sum_{\mu=1}^{4} n_{\tau\mu}$,故

$$\omega_E = \frac{\varepsilon}{(n_\tau + 2)\hbar} = \frac{e^2}{(n_\tau + 2)\hbar}. \tag{7}$$

令[9]

$$L_i = \frac{1}{2}(a^+ \sigma_i a + b^+ \sigma_i b), \tag{8}$$

其中 $a \equiv \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}$, $b \equiv \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}$, $a^+ \equiv (a_1^+ \quad a_2^+)$, $b^+ \equiv (b_1^+ \quad b_2^+)$, σ_i 是泡利矩阵,

$$a_1^+ = \frac{1}{\sqrt{2}}(\tau_1^+ + \mathrm{i}\tau_2^+),$$

$$a_1 = \frac{1}{\sqrt{2}}(\hat{\tau}_1 - \mathrm{i}\hat{\tau}_2),$$

$$a_2^+ = \frac{1}{\sqrt{2}}(\tau_3^+ - \mathrm{i}\tau_4^+),$$

$$a_2 = \frac{1}{\sqrt{2}}(\hat{\tau}_3 + \mathrm{i}\hat{\tau}_4),$$

$$b_1^+ = -\frac{1}{\sqrt{2}}(\tau_3^+ + \mathrm{i}\tau_4^+),$$

$$b_1 = -\frac{1}{\sqrt{2}}(\hat{\tau}_3 - \mathrm{i}\hat{\tau}_4),$$

$$b_2^+ = \frac{1}{\sqrt{2}}(\tau_1^+ - \mathrm{i}\tau_2^+),$$

$$b_2 = \frac{1}{\sqrt{2}}(\hat{\tau}_1 + \mathrm{i}\hat{\tau}_2). \tag{9}$$

再令 $\hat{n}_{ai} = a_i^+ a_i$, $\hat{n}_a = \hat{n}_{a1} + \hat{n}_{a2}$, $\hat{n}_{bi} = b_i^+ b_i$, $\hat{n}_b = \hat{n}_{b1} + \hat{n}_{b2}$,可证

$$\hbar_E = \sum \hbar\omega_E\left(\hat{n}_\mu + \frac{1}{2}\right) = \hbar\omega_E(\hat{n}_a + \hat{n}_b + 2), \tag{10}$$

$$[L_i \quad L_j] = \mathrm{i}\varepsilon_{ijk}L_k, \tag{11}$$

$$\hat{n}_a - \hat{n}_b = \mathrm{i}[\tau_2^+\hat{\tau}_1 - \tau_1^+\hat{\tau}_2 + \tau_3^+\hat{\tau}_4 - \tau_4^+\hat{\tau}_3] = 0. \tag{12}$$

由(11)式,L_i 构成 $SO(3)$李代数. 又可证得 $\hbar_E$, L^2, L_3 彼此对易,因而可令 $|n_a, n_b\rangle = |n_{a1}\, n_{a2}\, n_{b1}\, n_{b2}\rangle$为 $\hbar_E$, L^2, L_3 共同的本征函数,并有

$$\hat{n}_{ai}|n_a, n_b\rangle = n_{ai}|n_a, n_b\rangle,$$

$$\hat{n}_{bi}|n_a, n_b\rangle = n_{bi}|n_a, n_b\rangle, \tag{13}$$

$$\hbar_E|n_a, n_b\rangle = \hbar\omega_E(n_a + n_b + 2)|n_a n_b\rangle. \tag{14}$$

由(12)式,$n_a = n_b$,令 $n = n_a + 1 = n_b + 1$,有 $\hbar_E|n_a n_b\rangle = 2\hbar\omega_E n|n_a n_b\rangle$. 又由(6) h_E 的本征值为 $\hbar\omega_E(n_\tau + 1)$,而 $\omega_E = \left(-\frac{2E}{M}\right)^{1/2}$, $M = 4m$,可得氢原子能量本征值 $E_n = -\frac{me^4}{2n^2\hbar^2}$,其中 $n = \frac{n_\tau + 2}{2}$ 是整数.

3. 氢原子能量本征矢的玻色子表示

由于

$$L_3|n_a n_b\rangle = \frac{1}{2}[(n_{a_1} - n_{a_2}) + (n_{b_1} - n_{b_2})]|n_a n_b\rangle, \tag{15}$$

可见 $n_{a_2} = n_{b_2} = 0$ 时,$|n_a n_b\rangle$是 $m = l = \frac{1}{2}(n_{a_1} + n_{b_1})$状态,因此用$|n(= n_a + 1 = n_b + 1)lm\rangle$来标记 h_E, L^2 和 L_3 的共同本征态. 由 $n_{a_1} = n_{b_1} = l$,可见

$$|n = l + 1, ll\rangle = P_1^{+l}|0\rangle_n, \tag{16}$$

其中 $P_1^+ \equiv a_1^+ b_1^+$, $|0\rangle_n$ 满足 $a_i|0\rangle_n = b_i|0\rangle_n = 0$, $i = 1, 2$ 或 $\hat{\tau}_\mu|0\rangle_n = 0$, $\mu = 1, 2, 3, 4$. 令

$$L_{+1} = \frac{1}{\sqrt{2}}(L_1 + \mathrm{i}L_2) = \frac{1}{\sqrt{2}}(a_1^+ a_2 + b_1^+ b_2),$$

$$L_{-1} = \frac{1}{\sqrt{2}}(L_1 - \mathrm{i}L_2) = \frac{1}{\sqrt{2}}(a_2^+ a_1 + b_2^+ b_1), \tag{17}$$

有

$$|n = l + 1, lm\rangle = (L_-)^{l-m}(a_1^+ b_1^+)^l|0\rangle_n. \tag{18}$$

对于$|n > l + 1, l, m\rangle$,再考虑用 $a^+ b^+$ 构成的角动量为零的对算子 P_0^+ 作用,其中 P_0^+ 应有 $L_3 P_0^+|0\rangle_n = 0$, $L_\pm P_0^+|0\rangle_n = 0$. 取

$$P_0^+ = \frac{1}{\sqrt{2}}(a_1^+ b_2^+ - a_2^+ b_1^+), \tag{19}$$

显然满足条件,于是未归一化的氢原子波函数可表示为

$$|nlm\rangle = (P_0^+)^{n-1-l}L_-^{l-m}(P_1^+)^l|0\rangle_n. \tag{20}$$

必需指出,(20)式的形式虽然和三维谐振子相同[10],但(20)式中的玻色算子 a^+, b^+ 和真空态$|0\rangle_n$ 却都是依赖能量 E 或量子数 n 的,因为 a^+, b^+ 是 τ_μ^+ 的线性组合,而 $\tau_\mu^+ = \frac{1}{\sqrt{2}}\left(\eta_\mu - \frac{\partial}{\partial\eta_\mu}\right)$,其中 η_μ 的标度因子$\sqrt{\frac{M\omega_E}{\hbar}}$是依赖 频率 $'\omega_E$ 的,即依赖能量或 n. 在同一能量下,不同的 μ,标度因子相同,可以统一地写为

$$\tau_n^+ = \frac{1}{\sqrt{2}}\left(\sqrt{\frac{M\omega_n}{\hbar}}s - \sqrt{\frac{\hbar}{M\omega_n}}\frac{\partial}{\partial s}\right)$$

(注意 η 和 s 都有四个分量), (21)

改变标度因子$\sqrt{\frac{M\omega_n}{\hbar}}\to\sqrt{\frac{M\omega_{n'}}{\hbar}}$,则

$$\tau_{n'}^{+}=\frac{1}{\sqrt{2}}\left(\sqrt{\frac{M\omega_{n'}}{\hbar}}s-\sqrt{\frac{\hbar}{M\omega_{n'}}}\frac{\partial}{\partial s}\right)$$
$$=\frac{1}{\sqrt{2}}\left(\sqrt{\frac{\omega_{n'}}{\omega_n}}\sqrt{\frac{M\omega_n}{\hbar}}s-\sqrt{\frac{\omega_n}{\omega_{n'}}}\sqrt{\frac{\hbar}{M\omega_n}}\frac{\partial}{\partial s}\right).\tag{22}$$

由(4)式有

$$\tau_{n'}^{+}=\frac{1}{\sqrt{2}}\left(\sqrt{\frac{\omega_{n'}}{\omega_n}}+\sqrt{\frac{\omega_n}{\omega_{n'}}}\right)\tau_n^{+}+\frac{1}{\sqrt{2}}\left(\sqrt{\frac{\omega_{n'}}{\omega_n}}-\sqrt{\frac{\omega_n}{\omega_{n'}}}\right)\hat{\tau}_n,$$
$$\hat{\tau}_{n'}=\frac{1}{\sqrt{2}}\left(\sqrt{\frac{\omega_{n'}}{\omega_n}}-\sqrt{\frac{\omega_n}{\omega_{n'}}}\right)\tau_n^{+}+\frac{1}{\sqrt{2}}\left(\sqrt{\frac{\omega_{n'}}{\omega_n}}+\sqrt{\frac{\omega_n}{\omega_{n'}}}\right)\tau_n.\tag{23}$$

这正好是一个 Bogoliubov 变换,令

$$U=e^{\frac{1}{2}\zeta(\tau_n^{+2}-\hat{\tau}_n^2)},$$
$$U^{+}=e^{-\frac{1}{2}\zeta(\tau_n^{+2}-\hat{\tau}_n^2)},\tag{24}$$

取 $e^{\zeta}=\sqrt{\frac{\omega_n}{\omega_{n'}}}$,即得

$$\tau_{n'}^{+}=U\tau_n^{+}U^{+}=(\mathrm{ch}\zeta)\tau_n^{+}-(\mathrm{sh}\zeta)\hat{\tau}_n,$$
$$\hat{\tau}_{n'}=U\hat{\tau}_nU^{+}=(\mathrm{ch}\zeta)\hat{\tau}_n-(\mathrm{sh}\zeta)\tau_n^{+}.\tag{25}$$

因此只需在(20)式前面乘以 U 就可把标度因子从$\sqrt{\frac{M\omega_n}{\hbar}}\to\sqrt{\frac{M\omega_{n'}}{\hbar}}$.

$$U\prod_i\tau_n^{(i)+}|0\rangle_n=\prod_i(U\tau_n^{(i)+}U^{+})U|0\rangle_n$$
$$=\prod_i\tau_{n'}^{(i)+}|0\rangle_{n'},\tag{26}$$

$|0\rangle_{n'}$ 满足 $\tau_{n'}|0\rangle_{n'}=0$. 取基态($n=1$)的频率作为标度因子,$\sqrt{\frac{M\omega_E}{\hbar}}=\sqrt{\frac{2me^2}{\hbar^2}}$,另记 $n'=n$,$e^{\zeta}=\sqrt{\frac{\omega_1}{\omega_n}}=\sqrt{n}$,这时(20)式表为

$$|nlm\rangle=U_n(P_0^{+})^{n-1-l}L_{-}^{l-m}(P_1^{+})^{l}|0\rangle.\tag{27}$$

这里玻色算子的标度因子均为$\sqrt{\frac{M\omega}{\hbar}}=\sqrt{\frac{2me^2}{\hbar^2}}$,其中

$$U_n=e^{\frac{1}{2}\zeta\sum_{\mu=1}^{4}(\tau_\mu^{+2}-\hat{\tau}_\mu^2)}=e^{\sqrt{2}\zeta(P_0^{+}-P_0)}.\tag{28}$$

必需指出的第二点是虽然 $\hbar_E=\hbar\omega_E(\hat{n}_a+\hat{n}_b+2)$ 只和 $\hat{n}_a+\hat{n}_b$ 有关,似乎束缚态的氢原子具有 $SU(4)$对称性,但由于条件 $\hat{n}_a=\hat{n}_b$ 的限制,氢原子不具有 $SU(4)$对称性,只有 $SU(2)\otimes SU(2)$即 $SO(4)$对称性.

4. 氢原子能量本征矢的坐标表示

由(8),(9),(4),(1)式

$$L_3=\frac{1}{2}(a_1^{+}a_1-a_2^{+}a_2+b_1^{+}b_1-b_2^{+}b_2)$$
$$=\frac{i}{2}\left(\eta_2\frac{\partial}{\partial\eta_1}-\eta_1\frac{\partial}{\partial\eta_2}+\eta_4\frac{\partial}{\partial\eta_3}-\eta_3\frac{\partial}{\partial\eta_4}\right)$$
$$=\xi_1\left(-i\frac{\partial}{\partial\xi_2}\right)-\xi_2\left(-i\frac{\partial}{\partial\xi_1}\right).\tag{29}$$

同理可得 $L_i=\varepsilon_{ijk}\xi_j\left(-i\frac{\partial}{\partial\xi_k}\right)$,$i=1,2,3$. 其中 $\xi_i=\frac{M\omega_E}{\hbar}r_i$,$r_i$ 是普通直角坐标($r_1=x$),因此 L_i 正是普通空间的角动量算符 L_x,L_y,L_z.

下面先给出$|0\rangle_n$ 的坐标表示 $\psi_{n0}(q)=\langle\eta|0\rangle_n$,由于

$$\hat{\tau}_\mu\psi_{n0}(q)=\left(\eta_\mu+\frac{\partial}{\partial\eta_\mu}\right)\psi_{n0}(q)=0,$$
$$\mu=1,2,3,4.\tag{30}$$

所以

$$\psi_{n0}(q)=e^{-\frac{1}{2}\sum_{\mu=1}^{4}\eta_\mu^2}=e^{-\frac{1}{2}\rho}=e^{-\frac{M\omega_E}{2\hbar}}.\tag{31}$$

注意到 $n_\tau+2=n_a+n_b+2=2n$,$\omega_E=\frac{e^2}{2n\hbar}$,$M=4m$,

$$\langle n|0\rangle_n=\psi_{n0}(q)=e^{-r/\left(n\frac{\hbar^2}{me^2}\right)}=e^{-r/a_n},\tag{32}$$

其中 $a_n\equiv n\frac{\hbar^2}{me^2}$. 再由(1)式的 $r_i\to\xi_i$,$s_\mu\to\eta_\mu$,有

$$\frac{\partial}{\partial\eta_\mu}=\sum_i f_{\mu i}(\eta)\frac{\partial}{\partial\xi_i},$$
$$\frac{\partial^2}{\partial\eta_\gamma\partial\eta_\mu}=\frac{\partial}{\partial\eta_\gamma}\sum_i f_{\mu i}(\eta)\frac{\partial}{\partial\xi_i}$$
$$=\sum_{ij}f_{\mu i}(\eta)f_{\gamma j}(\eta)\frac{\partial^2}{\partial\xi_j\partial\xi_i}$$
$$+\sum_i\left(\frac{\partial f_{\mu i}}{\partial\eta_\gamma}\right)\frac{\partial}{\partial\xi_i},\tag{33}$$

给出 $P_1^{+}=a_1^{+}b_1^{+}$ 的坐标表示,

$$P_1^{+}=a_1^{+}b_1^{+}$$
$$=-\frac{1}{2}(\tau_1^{+}+i\tau_2^{+})(\tau_3^{+}+i\tau_4^{+})$$
$$=-\frac{1}{4}\left[\frac{1}{2}\xi_1+(4-2\tau^2)\frac{\partial}{\partial\xi_1}-2\xi_1\nabla_\xi^2+4(\boldsymbol{\xi}\cdot\boldsymbol{\nabla}_\xi)\frac{\partial}{\partial\xi_1}\right]-\frac{i}{4}\left[\frac{1}{2}\xi_2+(4-2\tau^2)\frac{\partial}{\partial\xi_2}-2\xi_2\nabla_\xi^2+4(\boldsymbol{\xi}\cdot\boldsymbol{\nabla}_\xi)\frac{\partial}{\partial\xi_2}\right]$$

$$= -\frac{1}{4}\left\{\sin\theta e^{i\varphi}\left[\frac{\rho}{2} + 2\rho\frac{\partial^2}{\partial\rho^2} - 2\rho\frac{\partial}{\partial\rho} + \frac{2}{\rho}L^2 + \left(2 - 4\frac{\partial}{\partial\rho}\right)L_3\right] + \left(4 - 2\rho + 4\rho\frac{\partial}{\partial\rho}\right)\frac{\cos\theta}{\rho}\sqrt{2}L_{+1}(\theta,\varphi)\right\}, \quad (34)$$

$$a_1^+ b_1^+ \langle\eta|0\rangle_n = a_1^+ b_1^+ e^{-\frac{1}{2}\rho} = -\frac{\rho}{2}e^{-\frac{\rho}{2}}Y_{11}(\theta,\varphi), \quad (35)$$

$$(a_1^+ b_1^+)^l\langle\eta|0\rangle_n = \left(-\frac{1}{4}\right)^l Y_{ll}(\theta,\varphi)\left(\sum_{k=1}^{l}\hat{O}_k\right)e^{-\frac{\rho}{2}}, \quad (36)$$

$$\hat{O}_k \equiv \frac{\rho}{2} + 2\rho\frac{\partial^2}{\partial\rho^2} - 2\rho\frac{\partial}{\partial\rho} + \frac{2}{\rho}k(k-1) + \left(2 - 4\frac{\partial}{\partial\rho}\right)(k-1). \quad (37)$$

用归纳法可证

$$\left(\prod_{k=1}^{l}\hat{O}_k\right)e^{-\frac{\rho}{2}} = \left(-\frac{\rho}{2}\right)^l e^{-\frac{\rho}{2}}. \quad (38)$$

于是

$$P_1^{+l}\langle\eta|0\rangle_n = \left(-\frac{\rho}{2}\right)^l e^{-\frac{\rho}{2}}Y_{11}(\theta,\varphi), \quad (39)$$

$$P_0^+ = \frac{1}{\sqrt{2}}(a_1^+ b_2^+ - a_2^+ b_1^+) = \frac{1}{4\sqrt{2}}\left[\eta^2 - 2\sum_{\mu=1}^{4}\eta_\mu\frac{\partial}{\partial\eta_\mu} - 4 + \Box_\tau\right] = \frac{1}{4\sqrt{2}}\left[4\rho\frac{\partial^2}{\partial\rho^2} + (8 - 4\rho)\frac{\partial}{\partial\rho^2} + \rho - \frac{4}{\rho}L^2 - 4\right], \quad (40)$$

$$P_0^+\rho^l e^{-\frac{\rho}{2}}Y_{ll}(\theta,\varphi) = \frac{1}{\sqrt{2}}\left[\rho\frac{\partial^2}{\partial\rho^2} + (2-\rho)\frac{\partial}{\partial\rho} + \frac{4}{\rho} - \frac{l(l+1)}{\rho} - 1\right]\rho^l e^{-\frac{\rho}{2}}Y_{ll}(\theta,\varphi)$$
$$= \frac{1}{\sqrt{2}}Y_{ll}(\theta,\varphi)\rho^l e^{-\frac{\rho}{2}}\left\{\rho\frac{\partial^2}{\partial\rho^2} - [2\rho - 2(l+1)]\frac{\partial}{\partial\rho} + \rho - 2(l+1)\right\}\cdot 1$$
$$= \frac{1}{\sqrt{2}}Y_{ll}(\theta,\varphi)\rho^l e^{-\frac{\rho}{2}}[-\hat{R}_\alpha(2l+2,\rho)]\cdot 1, \quad (41)$$

其中 $\hat{R}_\alpha(2l+2,\rho)$ 由算子 $\hat{R}_\alpha(\gamma,t) \equiv -t\frac{d^2}{dt^2} + (2t - \gamma)\frac{d}{dt} + (\gamma - t)$ 确定.

利用[14]

$$\langle\lambda\rangle_n = \frac{\Gamma(\lambda+n)}{\Gamma(\lambda)} = \lambda(\lambda+1)\cdots(\lambda+n-2)(\lambda+n-1),$$

合流超几何函数

$$F(\alpha,\gamma,t) = 1 + \sum_{n=1}\frac{(\alpha+n-1)(\alpha+n-2)\cdots(\alpha+1)\alpha}{n!(\gamma+n-1)(\gamma+n-2)\cdots(\gamma+1)\gamma}t^n = 1 + \sum_{n=1}\frac{\langle\alpha\rangle_n}{n!\langle\gamma\rangle_n}t^n, \quad (42)$$

显然有 $F(0,\gamma,t) = 1$，可以证明

$$\hat{R}_\alpha(\gamma,t)F(-n_\gamma,\gamma;t) = (\gamma + n_\gamma)F(-(n_\gamma+1),\gamma;t). \quad (43)$$

再由 $\hat{R}_\alpha^{n_\gamma}\cdot 1 = \langle\gamma\rangle_{n_\gamma}F(-n_\gamma,\gamma;t)$，可得未归一化的

$$\langle q|nll\rangle = (P_0^+)^{n-l-1}\rho^l e^{-\frac{\rho}{2}}Y_{ll} = \frac{1}{\sqrt{2}}Y_{ll}(\theta,\varphi)\rho^l e^{-\frac{\rho}{2}} \times [-R_\alpha(2l+2,\rho)]^{n-l-1}\cdot 1 = \frac{C}{\sqrt{2}}Y_{ll}(\theta,\varphi)\rho^l e^{-\frac{\rho}{2}} \times F(-(n-l-1),2(l+1);\rho), \quad (44)$$

其中 C 是常数. 最后得到未归一化的

$$\langle q|nlm\rangle = \psi_{nlm}(q) = (L_-)^{l-m}\langle q|nll\rangle = NY_{lm}(\theta,\varphi)\rho^l e^{-\frac{\rho}{2}} \times F(-(n-l-1),2(l+1);\rho). \quad (45)$$

(45)中无量纲 ρ 的标度因子 $\frac{M\omega_E}{\hbar} = \frac{2me^2}{n\hbar^2}$ 是与 n 有关，如果用 ρ_1 表示氢原子波函数中的 ρ，

$$\rho = \rho_1 = \frac{2me^2}{\hbar^2}r. \quad (46)$$

(45)式的 ρ 应写为 ρ_n，

$$\rho_n = \frac{2me^2}{n\hbar^2}r = \frac{\rho}{n}, \quad (47)$$

用 ρ 表示量子数为 n 的氢原子波函数，必需乘以重标度算子 U_n，由(27)式氢原子的波函数应为

$$\psi_{nlm}(q) = U_n\rho^l e^{-\frac{\rho}{2}} \times F(-(n-1-l),2(l+1);\rho)Y_{lm}(\theta,\varphi). \quad (48)$$

由(28)写出算子 U_n 的微分形式

$$U_n = e^{-\zeta\left(\sum_\mu\eta_\mu\frac{\partial}{\partial\eta_\mu}+2\right)} = e^{-2\zeta\left(\rho\frac{\partial}{\partial\rho}+1\right)} = e^{-2\zeta}e^{-2\zeta\rho\frac{\partial}{\partial\rho}}, \quad (49)$$

把 $\mathrm{e}^{-2\zeta}$ 并入归一化常数中,可取重标度算符为

$$\bar{U}_n = \mathrm{e}^{-2\zeta\rho\frac{\partial}{\partial\rho}}, \tag{50}$$

$$\begin{aligned}\bar{U}_n\rho &= \bar{U}_n\rho\bar{U}_n^{-1} \\ &= \mathrm{e}^{-2\zeta\rho\frac{\partial}{\partial\rho}}\rho\,\mathrm{e}^{2\zeta\rho\frac{\partial}{\partial\rho}} \\ &= \mathrm{e}^{-2\zeta\left[\rho\frac{\partial}{\partial\rho},\right]}\rho \\ &= \mathrm{e}^{-2\zeta}\rho = \frac{\rho}{n} = \rho_n,\end{aligned} \tag{51}$$

其中

$$\mathrm{e}^{[X,]}Y = 1 + \frac{1}{1!}[X,Y] + \frac{1}{2!}[X,[X,Y]] + \cdots, \tag{52}$$

所以

$$\bar{U}_n\rho^k = \bar{U}_n\rho^k\bar{U}_n^{-1} = (\bar{U}_n\rho\bar{U}_n^{-1})^k = \rho_n^k. \tag{53}$$

最后有

$$\begin{aligned}\varphi_{nlm}(q) &= \bar{U}_n\rho^l\mathrm{e}^{-\frac{\rho}{2}}F(-(n-1-l),\\ &\qquad 2(l+1);\rho)Y_{lm}(\theta,\varphi)\\ &= \Big((\bar{U}_n\rho^l\bar{U}_n^{-1})(\bar{U}_n\mathrm{e}^{-\frac{\rho}{2}}\bar{U}_n^{-1})\\ &\quad\times(\bar{U}_nF(-(n-1-l),2(l+1);\rho)\\ &\quad\times\bar{U}_n^{-1})U_nY_{lm}(\theta,\varphi)\\ &= \rho_n^l\mathrm{e}^{-\frac{\rho_n}{2}}F(-(n-1-l),\\ &\qquad 2(l+1);\rho)Y_{lm}(\theta,\varphi),\end{aligned} \tag{54}$$

其中 $\bar{U}_n$,ρ,ρ_n 分别由(50),(46)和(47)式给出.(54)式就是(27)式的坐标表示式.

5. 结 论

本文通过引入基态的玻色算子外加一个 Bogoliubov 变换,用代数方法解出氢原子能谱关系和波函数外,还给出了这些玻色算子跟坐标及其微分算子的关系,完满地解决了氢原子波函数的算子表示问题,也为其他量子可积或不可积系统的代数解法,提供了基础.

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Boson expression of hydrogen atom eigenfunction*

Li Xing-Hua† Yang Ya-Tian

(*School of Physics and Opto-Electronics Technology, Fujian Normal University, Fuzhou* 350007, *China*)

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Abstract

The eigenfunction of hydrogen atom is expressed in a unified way with four boson operators and Bogoliubov transformation, and the corresponding relations with the wave function expressed in spherical coordinates is given as well. The problem of operator expressions of hydrogen atoms is solved completely.

Keywords: boson expression, hydrogen atom, wave function

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† E-mail: xhli1@mail.china.com